



# Tricyclic graphs with maximum Merrifield–Simmons index<sup>☆</sup>

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## ABSTRACT

It is well known that the graph invariant, ‘the Merrifield–Simmons index’ is important one in structural chemistry. The connected acyclic graphs with maximal and minimal Merrifield–Simmons indices are determined by Prodinger and Tichy [H. Prodinger, R.F. Tichy, Fibonacci numbers of graphs, *Fibonacci Quart.* 20 (1982) 16–21]. The sharp upper and lower bounds for the Merrifield–Simmons indices of unicyclic graphs are characterized by Pedersen and Vestergaard [A.S. Pedersen, P.D. Vestergaard, The number of independent sets in unicyclic graphs, *Discrete Appl. Math.* 152 (2005) 246–256]. The sharp upper bound for the Merrifield–Simmons index of bicyclic graphs is obtained by Deng, Chen and Zhang [H. Deng, S. Chen, J. Zhang, The Merrifield–Simmons index in  $(n, n + 1)$ -graphs, *J. Math. Chem.* 43 (1) (2008) 75–91]. The sharp lower bound for the Merrifield–Simmons index of bicyclic graphs is determined by Jing and Li [W. Jing, S. Li, The number of independent sets in bicyclic graphs, *Ars Combin.* 2008 (in press)]. In this paper, we will consider the tricyclic graph, i.e., a connected graph with cyclomatic number 3. The tricyclic graph with  $n$  vertices having maximum Merrifield–Simmons index is determined.

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## 1. Introduction

Let  $G$  be a graph on  $n$  vertices. Two vertices of  $G$  are said to be *independent* if they are not adjacent in  $G$ . An *independent  $k$  set* is a set of  $k$  vertices, no two of which are adjacent. Denote by  $i(G, k)$  the number of the  $k$ -independent sets of  $G$ . It follows directly from the definition that  $\emptyset$  is an independent set. Then  $i(G, 0) = 1$  for any graph  $G$ . The *Merrifield–Simmons index* of  $G$ , denoted by  $i(G)$ , is defined as

$$i(G) = \sum_{k=0}^n i(G, k).$$

So  $i(G)$  is equal to the total number of independent sets of  $G$ . The total number of independent sets of a graph  $G$  is also called the *Fibonacci number* of the graph  $G$ . It was introduced in 1982 in a paper of Prodinger and Tichy [22].

The Merrifield–Simmons index  $i(G)$  [20] is one of the topological indices whose mathematical properties were studied in some detail [3, 11, 7–9] whereas its applicability for QSPR and QSAR was examined to a much lesser extent; in [20] it was shown that  $i(G)$  is correlated with the boiling points. Now there have been many papers studying the Merrifield–Simmons index. In [22], Prodinger and Tichy shown that, for  $n$ -vertex trees, the star has the maximal Merrifield–Simmons index and the path has the minimal Merrifield–Simmons index. In [1], Alameddine determined the sharp bounds for

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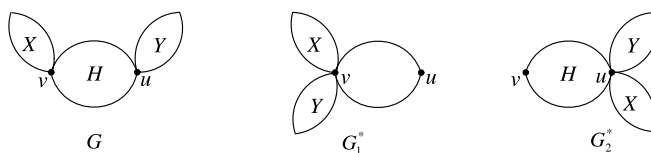


Fig. 1. Graphs  $G$ ,  $G_1^*$  and  $G_2^*$ .

the Merrifield–Simmons index of a maximal outer planar graph. Gutman [10], Zhang and Tian [27,28] studied the Merrifield–Simmons indices of hexagonal chains and catacondensed systems, respectively. Ren and Zhang [23] determined the minimal Merrifield–Simmons index of double hexagonal chains. In [17], Li et al. characterized the tree with the maximal Merrifield–Simmons index among the trees with given diameter. In [26], Yu and Tian studied the Merrifield–Simmons indices of the graphs with given edge-independence number and cyclomatic number. (For the definition of cyclomatic number of a graph one may refer to [2]). Yu and Lv [19,25] studied the Merrifield–Simmons indices of trees with maximal degree and given pendent vertices, respectively. Ye et al., ordered the unicyclic graphs with given girth according to the Merrifield–Simmons index in [24]. Pedersen and Vestergaard [21] determined upper and lower bounds for the number of independent sets in a unicyclic graph in terms of its order. Li and Zhu [18] determined the sharp upper bound for the number of independent sets in a unicyclic graph of a given diameter. In [4], Deng et al., determined the upper bounds for number of independent sets among bicyclic graphs, while Jing and one of the present authors determined the sharp lower bound for the number of independent sets in a bicyclic graph in terms of its order; see [12]. For detailed information on chemical applications, we refer to [11].

Just as above, the extremal Merrifield–Simmons index in the class of connected graphs with cyclomatic number 0, 1, 2 have been determined, respectively. It is then natural to consider the connected graphs with cyclomatic number 3, i.e., the set of tricyclic graphs. Furthermore, there have been some previous works for tricyclic graphs with a regular investigation both in total  $\pi$ -electron energies with the framework of the HMO approximation [14] and in the theory of graphic spectra and nullity of graphs; see [5,6,13].

A *tricyclic graph* is a connected graph with  $n$  vertices and  $n + 2$  edges. Let  $\mathcal{T}_n$  be the class of tricyclic graphs  $G$  on  $n$  vertices. In order to state our results, we introduce some notation and terminology. For other undefined notation we refer to Bollobás [2]. We only consider finite, simple and undirected graphs. If  $W \subseteq V(G)$ , we denote by  $G - W$  the subgraph of  $G$  obtained by deleting the vertices of  $W$  and the edges incident with them. Similarly, if  $E' \subseteq E(G)$ , we denote by  $G - E'$  the subgraph of  $G$  obtained by deleting the edges of  $E'$ . If  $W = \{v\}$  and  $E' = \{xy\}$ , we write  $G - v$  and  $G - xy$  instead of  $G - \{v\}$  and  $G - \{xy\}$ , respectively. We denote by  $P_n$ ,  $C_n$  and  $K_{1,n-1}$  the path, the cycle and the star on  $n$  vertices, respectively. Let  $G_1, G_2$  be two connected graphs with  $V(G_1) \cap V(G_2) = \{v\}$ , then let  $G = G_1 v G_2$  be a graph defined by  $V(G) = V(G_1) \cup V(G_2)$  and  $E(G) = E(G_1) \cup E(G_2)$ .

In this paper, we determine the upper bound for the Merrifield–Simmons index in a tricyclic graph in terms of its order, and we also characterize the corresponding extremal graph.

## 2. Lemmas

In this section, some necessary lemmas are given which will be used to prove our main results.

**Lemma 2.1** ([11]). Let  $G = (V, E)$  be a graph.

- (i) If  $uv \in E(G)$ , then  $i(G) = i(G - uv) - i(G - (N[u] \cup N[v]))$ ;
- (ii) If  $v \in V(G)$ , then  $i(G) = i(G - v) + i(G - N[v])$ ;
- (iii) If  $G_1, G_2, \dots, G_t$  are the components of the graph  $G$ , then  $i(G) = \prod_{j=1}^t i(G_j)$ .

Two graphs are said to be *disjoint* if they have no vertex in common.

**Lemma 2.2** ([15]). Let  $H, X, Y$  be three connected graphs disjoint in pairs. Suppose that  $u, v$  are two vertices of  $H$ ,  $v'$  is a vertex of  $X$ ,  $u'$  is a vertex of  $Y$ . Let  $G$  be the graph obtained from  $H, X, Y$  by identifying  $v$  with  $v'$  and  $u$  with  $u'$ , respectively. Let  $G_1^*$  be the graph obtained from  $H, X, Y$  by identifying vertices  $v, v', u'$  and  $G_2^*$  be the graph obtained from  $H, X, Y$  by identifying vertices  $u, v', u'$ ; see Fig. 1. Then

$$i(G_1^*) > i(G) \quad \text{or} \quad i(G_2^*) > i(G).$$

**Lemma 2.3** ([16]). Let  $H$  be a connected graph and  $T_l$  be a tree of order  $l + 1$  with  $V(H) \cap T_l = \{v\}$ . Then  $i(HvT_l) \leq i(HvK_{1,l})$ , the equality holds if, and only if,  $HvT_l \cong HvK_{1,l}$ , where  $v$  is identified with the center of the star  $K_{1,l}$  in  $HvK_{1,l}$ .

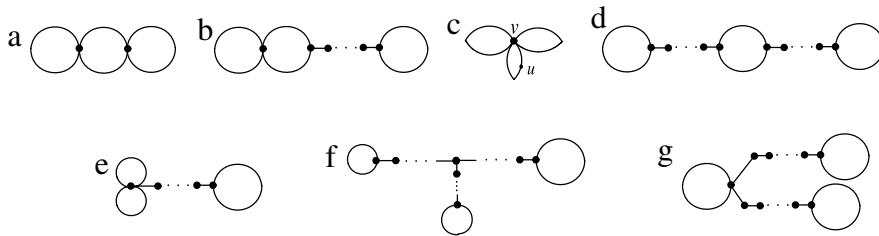


Fig. 2. Seven possible cases for the arrangement of three cycles contained in  $G$ .

According to the definition of the Merrifield–Simmons index of a graph  $G$ , by Lemma 2.1, if  $v$  is a vertex of  $G$ , then  $i(G) > i(G - v)$ . In particular, when  $v$  is a pendent vertex of  $G$  and  $u$  is the unique vertex adjacent to  $v$ , we have

$$i(G) = i(G - v) + i(G - \{u, v\}). \quad (2.1)$$

So it is easy to see that  $i(P_0) = 1$ ,  $i(P_1) = 2$  and  $i(P_n) = i(P_{n-1}) + i(P_{n-2})$  for  $n \geq 2$ . Let  $F_n$  be the  $n$ th Fibonacci number, defined by  $F_n = F_{n-1} + F_{n-2}$  with initial conditions  $F_0 = 1$  and  $F_1 = 1$ . Therefore,

$$i(P_n) = F_{n+1} = \frac{1}{\sqrt{5}} \left[ \left( \frac{1 + \sqrt{5}}{2} \right)^{n+2} - \left( \frac{1 - \sqrt{5}}{2} \right)^{n+2} \right].$$

Note that  $F_{n+m} = F_n F_m + F_{n-1} F_{m-1}$ . For convenience, we let  $F_n = 0$  for  $n < 0$ .

By [5,6,14] a tricyclic graph  $G$  contains at least 3 cycles and at most 7 cycles, furthermore, there do not exist 5 cycles in  $G$ . Then let  $\mathcal{T}_n = \mathcal{T}_n^3 \cup \mathcal{T}_n^4 \cup \mathcal{T}_n^6 \cup \mathcal{T}_n^7$ , where  $\mathcal{T}_n^i$  denotes the set of tricyclic graphs on  $n$  vertices with exact  $i$  cycles for  $i = 3, 4, 6, 7$ .

Let  $M$  be a graph formed by attaching three cycles  $C_a$ ,  $C_b$  and  $C_c$  to a common vertex  $v$ ; see Fig. 2(c). Then let  $G_{n,a,b,c}^k$  be a graph on  $n$  vertices created from  $M$  by attaching  $k$  pendent vertices to  $v$ , as well we set  $\mathcal{T}^* = \{G \in \mathcal{T}_n : G \text{ is a graph obtained from } M \text{ by attaching } k \text{ pendent vertices to one vertex except } v, \text{ say } u, \text{ on } M\}$ , where  $a + b + c + k = n + 2$ . For convenience, let  $\tilde{G}_{n,a,b,c}^k$  be any one of the members in  $\mathcal{T}^*$ .

At first we shall show that the Merrifield–Simmons index of any member in  $\mathcal{T}^*$  is less than that of  $G_{n,a,b,c}^k$ . In fact, by Lemma 2.2, the following lemma is immediate.

**Lemma 2.4.**  $i(\tilde{G}_{n,a,b,c}^k) < i(G_{n,a,b,c}^k)$ .

**Lemma 2.5.** Let  $G$  be an  $n$ -vertex tricyclic graph possessing exactly three cycles, say  $C_a$ ,  $C_b$  and  $C_c$ , then  $i(G) \leq i(G_{n,a,b,c}^k)$ .

**Proof.** Let  $G$  be an  $n$ -vertex tricyclic graph processing exactly three cycles. The arrangement of the three cycles contained in  $G$  is depicted in Fig. 2; see [5,6,14]. Then repeatedly using Lemmas 2.2 and 2.3, we have either

$$i(G) \leq i(G_{n,a,b,c}^k) \quad \text{or} \quad i(G) \leq i(\tilde{G}_{n,a,b,c}^k).$$

Hence, in view of Lemma 2.4, we have  $i(G) \leq i(G_{n,a,b,c}^k)$ , as desired.  $\square$

**Lemma 2.6.** For positive integers  $a, b, c, k$ ,

- (i)  $i(G_{n,a,b,c}^k) < i(G_{n,a-1,b,c}^{k+1})$  for  $a \geq 4, b, c \geq 3$ .
- (ii)  $i(G_{n,a,b,c}^k) < i(G_{n,a,b-1,c}^{k+1})$  for  $b \geq 4, a, c \geq 3$ .
- (iii)  $i(G_{n,a,b,c}^k) < i(G_{n,a,b,c-1}^{k+1})$  for  $c \geq 4, a, b \geq 3$ .

**Proof.** By the symmetry of three cycles  $C_a$ ,  $C_b$  and  $C_c$  contained in  $G$ , here we only show that (i) holds. We omit the proofs for (ii) and (iii). Choose a pendent vertex, say  $v$ , in  $G_{n,a,b,c}^k$  (respectively,  $G_{n,a-1,b,c}^{k+1}$ ), then repeated using Eq. (2.1), we get

$$\begin{aligned} i(G_{n,a-1,b,c}^{k+1}) - i(G_{n,a,b,c}^k) &= 2^k(2F_{a-1}F_bF_c - F_aF_bF_c) + F_{a-3}F_{b-2}F_{c-2} - F_{a-2}F_{b-2}F_{c-2} \\ &= 2^k[2F_{a-1}F_bF_c - (F_{a-1} + F_{a-2})F_bF_c] + F_{a-3}F_{b-2}F_{c-2} - (F_{a-3} + F_{a-4})F_{b-2}F_{c-2} \\ &= 2^k(F_{a-1}F_bF_c - F_{a-2}F_bF_c) - F_{a-4}F_{b-2}F_{c-2} \\ &= 2^k(F_{a-1} - F_{a-2})F_bF_c - F_{a-4}F_{b-2}F_{c-2} \\ &= 2^kF_{a-3}F_bF_c - F_{a-4}F_{b-2}F_{c-2} \\ &\geq 2F_{a-3}F_bF_c - F_{a-4}F_{b-2}F_{c-2} \\ &> 0. \end{aligned}$$

The last inequality follows by  $a \geq 4, b, c \geq 3$ . This completes the proof of Lemma 2.6.  $\square$

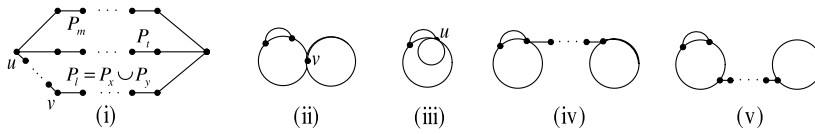


Fig. 3. (i) is the graph  $B_1$  and (ii), (iii), (iv), (v) are the four types of  $\tilde{G}$ -graphs.

Let  $P_l, P_m, P_t$  be three vertex-disjoint paths, where  $l, m, t \geq 2$  and at most one of them is 2. Identifying the three initial vertices and terminal vertices of them, respectively, the resulting graph, denoted by  $B_1$ , is called a  $\theta$ -graph; see Fig. 3(i). Furthermore, let  $C_b$  be a cycle. Connect  $C_b$  and  $B_1$  by a path  $P_s$ , where  $s \geq 1$  and call the resulting graph  $\tilde{G}$ -graph. By [5,6,14], we know that there are exactly four types of  $\tilde{G}$ -graph; see Fig. 3(ii)–(v). Furthermore,  $\mathcal{T}_n^4$  is a set of graphs each of which is a  $\tilde{G}$ -graph, has some trees attached, if possible.

For convenience, let  $C_a, C_c$  and  $C_d$  be the three cycles contained in  $B_1$ , where  $C_a = P_l \cup P_m$ ,  $C_c = P_m \cup P_t$ ,  $C_d = P_t \cup P_l = P_t \cup P_x \cup P_y$ ; see Fig. 3(i). Set

$$G_1 := B_1 u C_b, \quad G_2 := B_1 v C_b. \quad (2.2)$$

Thus, we define two tricyclic graphs in  $\mathcal{T}_n^4$  as follows:

- $A_{m,l,b,t}^k$  is an  $n$ -vertex tricyclic graph formed from  $G_1$  by attaching  $k$  pendent vertices to  $u$ .
- $\bar{A}_{m,b,t}^{k,x,y}$  is an  $n$ -vertex tricyclic graph created from  $G_2$  by attaching  $k$  pendent vertices to  $v$ .

In the above two graphs, the number of pendent vertices is in fact  $n + 5 - m - l - t - b$ , i.e.,  $k = n + 5 - m - l - t - b$ .

**Lemma 2.7.** Let  $G$  be in  $\mathcal{T}_n^4$  such that  $G$  contains the  $\theta$ -graph  $B_1$  and a cycle  $C_b$  with  $E(B_1) \cap E(C_b) = \emptyset$ . Then  $i(G) \leq i(A_{m,l,b,t}^{k'})$ , the equality holds if and only if  $G \cong A_{m,l,b,t}^{k'}$ , where  $k' = n - (|V(B_1)| + |V(C_b)| - 1)$ .

**Proof.** We distinguish the following two possible cases to prove this lemma.

Case 1.  $k' = 0$ . In this case, it is sufficient for us to consider two graphs  $G_1, G_2$  defined in (2.2). Note that in  $B_1$ ,  $l = x + y - 1$ , hence repeated using Lemma 2.1, we obtain

$$\begin{aligned} i(G_1) &= F_b(F_{x-1}F_{y-1}F_{m-1}F_{t-1} + F_{x-2}F_{y-2}F_{m-1}F_{t-1} + F_{x-1}F_{y-2}F_{m-2}F_{t-2} \\ &\quad + F_{x-2}F_{y-3}F_{m-2}F_{t-2}) + F_{b-2}(F_{l-2}F_{m-2}F_{t-2} + F_{l-3}F_{m-3}F_{t-3}), \\ i(G_2) &= F_b(F_{x-1}F_{y-1}F_{t-1}F_{m-1} + F_{x-1}F_{y-2}F_{t-2}F_{m-2} + F_{x-2}F_{y-2}F_{t-3}F_{m-3} + F_{x-2}F_{y-1}F_{t-2}F_{m-2}) \\ &\quad + F_{b-2}(F_{x-2}F_{y-2}F_{t-1}F_{m-1} + F_{x-2}F_{y-3}F_{t-2}F_{m-2} + F_{x-3}F_{y-2}F_{t-2}F_{m-2} + F_{x-3}F_{y-3}F_{t-3}F_{m-3}). \end{aligned}$$

Thus,

$$i(G_1) - i(G_2) = F_{b-1}(F_{x-2}F_{y-2}F_{t-2}F_{m-3} + F_{x-2}F_{y-2}F_{t-3}F_{m-2}).$$

Note that  $mt \geq 6$ , therefore  $F_{b-1}(F_{x-2}F_{y-2}F_{t-2}F_{m-3} + F_{x-2}F_{y-2}F_{t-3}F_{m-2}) > 0$ , i.e.,  $i(G_1) > i(G_2)$ . Hence when  $k' = 0$ , we have  $i(G) \leq i(G_1) = i(A_{m,l,b,t}^0)$ , the equality holds if and only if  $G \cong A_{m,l,b,t}^0$ .

Case 2.  $k' \geq 1$ . In this case, by applying Lemmas 2.2 and 2.3 repeatedly, we have

$$i(G) \leq i(A_{m,l,b,t}^{k'}), \quad \text{or} \quad i(G) \leq i(\bar{A}_{m,b,t}^{k',x,y}).$$

We are to show that  $i(\bar{A}_{m,b,t}^{k',x,y}) < i(A_{m,l,b,t}^{k'})$ . In fact, denote all the pendent vertices in  $A_{m,l,b,t}^{k'}$  by  $v_1, v_2, \dots, v_{k'}$ . Then let  $T_1 = A_{m,l,b,t}^{k'} - \{u, v_1, \dots, v_{k'}\} - V(C_b)$ ,  $T'_1 = T_1 - N[u]$ . Thus

$$\begin{aligned} i(A_{m,l,b,t}^{k'}) &= i(A_{m,l,b,t}^{k'} - v_1) + i(A_{m,l,b,t}^{k'} - N[v_1]) \\ &= i(A_{m,l,b,t}^{k'-1}) + i(P_{b-1} \cup T_1 \cup \{v_2, \dots, v_{k'}\}) \\ &= i(A_{m,l,b,t}^{k'-1}) + 2^{k'-1}F_b i(T_1) \\ &= \dots \\ &= i(A_{m,l,b,t}^0) + 2^0F_b i(T_1) + \dots + 2^{k'-1}F_b i(T_1) \\ &= 2^{k'}F_b i(T_1) + F_{b-2}i(T'_1), \end{aligned}$$

where

$$\begin{aligned} i(T_1) &= i(T_1 - w) + i(T_1 - N[w]) \\ &= i(P_{l-2} \cup P_{t-2} \cup P_{m-2}) + i(P_{l-3} \cup P_{t-3} \cup P_{m-3}) \\ &= F_{l-1}F_{t-1}F_{m-1} + F_{l-2}F_{t-2}F_{m-2}, \\ i(T'_1) &= F_{l-2}F_{t-2}F_{m-2} + F_{l-3}F_{t-3}F_{m-3} \end{aligned}$$

and so

$$i(A_{m,l,b,t}^k) = 2^k F_b(F_{l-1}F_{t-1}F_{m-1} + F_{l-2}F_{t-2}F_{m-2}) + F_{b-2}(F_{l-2}F_{t-2}F_{m-2} + F_{l-3}F_{t-3}F_{m-3}).$$

Similarly,

$$i(\bar{A}_{m,b,t}^{k',x,y}) = 2^{k'} F_b[F_{x-1}(F_{y-1}F_{t-1}F_{m-1} + F_{y-2}F_{t-2}F_{m-2}) + F_{x-2}(F_{y-2}F_{t-3}F_{m-3} + F_{y-1}F_{t-2}F_{m-2})] \\ + F_{b-2}[F_{x-2}(F_{y-2}F_{t-1}F_{m-1} + F_{y-3}F_{t-2}F_{m-2}) + F_{x-3}(F_{y-2}F_{t-2}F_{m-2} + F_{y-3}F_{t-3}F_{m-3})].$$

Hence,

$$i(A_{m,l,b,t}^{k'}) - i(\bar{A}_{m,b,t}^{k',x,y}) = 2^{k'} F_b[F_{x-2}F_{y-2}(F_{t-1}F_{m-1} - F_{t-3}F_{m-3}) + (F_{x-2}F_{y-3} - F_{x-2}F_{y-1})F_{t-2}F_{m-2}] \\ + F_{b-2}[(F_{x-1}F_{y-2} - F_{x-3}F_{y-2})F_{t-2}F_{m-2} + F_{x-2}F_{y-2}(F_{t-3}F_{m-3} - F_{t-1}F_{m-1})] \\ \geq 2F_b[F_{x-2}F_{y-2}(F_{t-1}F_{m-1} - F_{t-3}F_{m-3}) + (F_{x-2}F_{y-3} - F_{x-2}F_{y-1})F_{t-2}F_{m-2}] \\ + F_{b-2}[(F_{x-1}F_{y-2} - F_{x-3}F_{y-2})F_{t-2}F_{m-2} + F_{x-2}F_{y-2}(F_{t-3}F_{m-3} - F_{t-1}F_{m-1})] \\ = 2F_{b-1}F_{x-2}F_{y-2}(F_{t-1}F_{m-1} - F_{t-2}F_{m-2} - F_{t-3}F_{m-3}) \\ + F_{b-2}F_{x-2}F_{y-2}(F_{t-1}F_{m-1} - F_{t-2}F_{m-2} - F_{t-3}F_{m-3}) \\ = F_{x-2}F_{y-2}(F_{t-1}F_{m-1} - F_{t-2}F_{m-2} - F_{t-3}F_{m-3})(2F_{b-1} + F_{b-2}) \\ = F_{x-2}F_{y-2}(F_{t-3}F_{m-2} + F_{t-2}F_{m-3})(2F_{b-1} + F_{b-2}).$$

Note that  $b \geq 3$ ,  $x, y, t, m \geq 2$  and if  $t = 2$  (or  $m = 2$ ), then  $m \geq 3$  (or  $t \geq 3$ ), otherwise the resulting graph is not a simple graph. Therefore, we obtain  $F_{x-2}F_{y-2}(F_{t-3}F_{m-2} + F_{t-2}F_{m-3})(2F_{b-1} + F_{b-2}) > 0$ , i.e.,  $i(\bar{A}_{m,b,t}^{k',x,y}) < i(A_{m,l,b,t}^{k'})$ . That is to say,  $i(G) \leq i(A_{m,l,b,t}^{k'})$ , the equality holds if and only if  $G \cong A_{m,l,b,t}^{k'}$ .

By Cases 1 and 2, we complete the proof of Lemma 2.7.  $\square$

**Lemma 2.8.** For positive integers  $m, l, b, t, k$ ,

- (i)  $i(A_{m,l-1,b,t}^{k+1}) > i(A_{m,l,b,t}^k)$  for either  $l \geq 4, b \geq 3, m, t \geq 2$  and  $mt \geq 6$ , or  $l = 3, b, m, t \geq 3$ .
- (ii)  $i(A_{m-1,l,b,t}^{k+1}) > i(A_{m,l,b,t}^k)$  for either  $m \geq 4, b \geq 3, l, t \geq 2$  and  $lt \geq 6$ , or  $m = 3, b, l, t \geq 3$ .
- (iii)  $i(A_{m,l,b-1,t}^{k+1}) > i(A_{m,l,b,t}^k)$  for  $b \geq 4, l, m, t \geq 2$  and  $lmt \geq 18$ .
- (iv)  $i(A_{m,l,b,t-1}^{k+1}) > i(A_{m,l,b,t}^k)$  for either  $t \geq 4, b \geq 3, l, t \geq 2$  and  $lt \geq 6$ , or  $t = 3, m, l, b \geq 3$ .

**Proof.** (i) When  $l \geq 4, b \geq 3, m, t \geq 2$  and  $mt \geq 6$ , by Lemma 2.7, we have

$$i(A_{m,l-1,b,t}^{k+1}) - i(A_{m,l,b,t}^k) = 2^{k+1} F_b(F_{l-2}F_{t-1}F_{m-1} + F_{l-3}F_{t-2}F_{m-2}) + F_{b-2}(F_{l-3}F_{t-2}F_{m-2} + F_{l-4}F_{t-3}F_{m-3}) \\ - [2^k F_b(F_{l-1}F_{t-1}F_{m-1} + F_{l-2}F_{t-2}F_{m-2}) + F_{b-2}(F_{l-2}F_{t-2}F_{m-2} + F_{l-3}F_{t-3}F_{m-3})] \\ = 2^k F_b F_{l-4}F_{t-1}F_{m-1} - F_{b-2}F_{l-4}F_{t-2}F_{m-2} + 2^k F_b F_{l-5}F_{t-2}F_{m-2} - F_{b-2}F_{l-5}F_{t-3}F_{m-3}.$$

Note that  $l \geq 4, b \geq 3, m, t \geq 2$  and  $mt \geq 6$ , thereby,

$$2^k F_b F_{l-4}F_{t-1}F_{m-1} - F_{b-2}F_{l-4}F_{t-2}F_{m-2} + 2^k F_b F_{l-5}F_{t-2}F_{m-2} - F_{b-2}F_{l-5}F_{t-3}F_{m-3} > 0,$$

and so,  $i(A_{m,l-1,b,t}^{k+1}) > i(A_{m,l,b,t}^k)$  holds in this case.

When  $l = 3, b, m, t \geq 3$ , by Lemma 2.7, we have

$$i(A_{m,2,b,t}^{k+1}) - i(A_{m,3,b,t}^k) = 2^{k+1} F_b(F_{t-1}F_{m-1} + F_{t-2}F_{m-2}) + F_{b-2}(F_{t-2}F_{m-2}) \\ - [2^k F_b(F_{t-1}F_{m-1} + F_{t-2}F_{m-2}) + F_{b-2}(F_{t-2}F_{m-2} + F_{t-3}F_{m-3})] \\ = 2^k F_b F_{t-2}F_{m-2} - F_{b-2}F_{t-3}F_{m-3} > 0,$$

that is to say,  $i(A_{m,l-1,b,t}^{k+1}) > i(A_{m,l,b,t}^k)$  for  $l = 3, b, m, t \geq 3$ . Thus (i) holds.

With the same method as in (i), we can also show that (ii)–(iv) are true. We omit the procedure here. This completes the proof of Lemma 2.8.  $\square$

We know from [5,6,14] that if tricyclic graph has six cycles, then the arrangement of these cycles has three forms; see Fig. 4. Then define four tricyclic graphs in  $\mathcal{T}_n^6$  as follows:

- $H_{m,l,b,c}^k$  is a tricyclic graph with exact six cycles on  $n$  vertices created from Fig. 4(I) by attaching  $k$  pendent vertices to  $v$ , where  $m + l + b + c + k = n + 6$  and  $P_m = P_x \cup P_y$ .
- $\bar{H}_{m,l,b,c}^{k,x,y}$  is any member of the set of  $n$ -vertex tricyclic graphs with exact six cycles created from Fig. 4(I) by attaching  $k$  pendent vertices to  $u$  ( $\neq v, w$ ), where  $m + l + b + c + k = n + 6$  and  $P_m = P_x \cup P_y$ .
- $Q_{c,t_1,t_2}^k$  is a tricyclic graph with exact six cycles on  $n$  vertices created from Fig. 4(II) by attaching  $k$  pendent vertices to  $v$ , where  $c + t_1 + t_2 + k = n + 3$ .

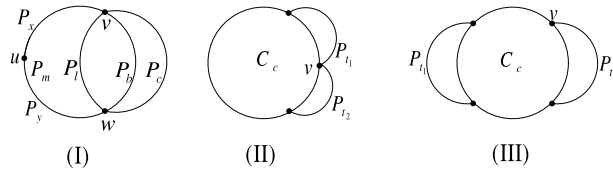


Fig. 4. Three possible forms for the arrangement of six cycles in tricyclic graphs.

- $S_{c,t_1,t_2}^k$  is a tricyclic graph with exact six cycles on  $n$  vertices created from Fig. 4(III) by attaching  $k$  pendent vertices to  $v$ , where  $c + t_1 + t_2 + k = n + 4$ .

**Lemma 2.9.** Let  $G \in \mathcal{T}_n^6$ .

- If the six cycles in  $G$  are the same as Fig. 4(I), then we have  $i(G) \leq i(H_{m,l,b,c}^k)$ .
- If the six cycles in  $G$  are the same as Fig. 4(II), then we have  $i(G) \leq i(Q_{c,t_1,t_2}^k)$ .
- If the six cycles in  $G$  are the same as Fig. 4(III), then we have  $i(G) \leq i(S_{c,t_1,t_2}^k)$ .

**Proof.** (a) For any graph  $G$  in  $\mathcal{T}_n^6$ , if the arrangement of six cycles in  $G$  is the same as that of Fig. 4(I) and  $G \not\cong H_{m,l,b,c}^k, \bar{H}_{m,l,b,c}^{k,x,y}$ , repeated applications of Lemmas 2.2 and 2.3 give

$$i(G) < i(H_{m,l,b,c}^k) \quad \text{or} \quad i(G) < i(\bar{H}_{m,l,b,c}^{k,x,y}).$$

In order to complete the proof of (a), it suffices to show that  $i(\bar{H}_{m,l,b,c}^{k,x,y}) < i(H_{m,l,b,c}^k)$  holds. For convenience, let  $v_1, v_2, \dots, v_k$  be the  $k$  pendent vertices of  $H_{m,l,b,c}^k$ , then set  $T_1 = H_{m,l,b,c}^k - \{v, v_1, \dots, v_k\}$  and  $T'_1 = T_1 - N[v]$ . By Lemma 2.1, we have

$$\begin{aligned} i(H_{m,l,b,c}^k) &= i(H_{m,l,b,c}^k - v_1) + i(H_{m,l,b,c}^k - N[v_1]) \\ &= i(H_{m,l,b,c}^k - v_1) + i(T_1 \cup \{v_2, \dots, v_k\}) \\ &= i(H_{m,l,b,c}^k - v_1) + 2^{k-1}i(T_1) \\ &= \dots \\ &= i(H_{m,l,b,c}^k - v_1 - \dots - v_k) + 2^0i(T_1) + \dots + 2^{k-1}i(T_1) \\ &= i(H_{m,l,b,c}^0) + 2^0i(T_1) + \dots + 2^{k-1}i(T_1) \\ &= 2^k i(T_1) + i(T'_1), \end{aligned}$$

where

$$\begin{aligned} i(T_1) &= i(T_1 - w) + i(T_1 - N[w]) \\ &= i(P_{l-2} \cup P_{m-2} \cup P_{b-2} \cup P_{c-2}) + i(P_{l-3} \cup P_{m-3} \cup P_{b-3} \cup P_{c-3}) \\ &= F_{l-1}F_{m-1}F_{b-1}F_{c-1} + F_{l-2}F_{m-2}F_{b-2}F_{c-2}, \\ i(T'_1) &= F_{l-2}F_{m-2}F_{b-2}F_{c-2} + F_{l-3}F_{m-3}F_{b-3}F_{c-3} \end{aligned}$$

and so

$$i(H_{m,l,b,c}^k) = 2^k(F_{l-1}F_{m-1}F_{b-1}F_{c-1} + F_{l-2}F_{m-2}F_{b-2}F_{c-2}) + F_{l-2}F_{m-2}F_{b-2}F_{c-2} + F_{l-3}F_{m-3}F_{b-3}F_{c-3}. \quad (2.3)$$

Similarly,

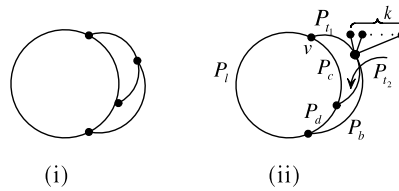
$$\begin{aligned} i(\bar{H}_{m,l,b,c}^{k,x,y}) &= 2^k[F_{x-1}(F_{y-1}F_{m-1}F_{b-1}F_{c-1} + F_{y-2}F_{m-2}F_{b-2}F_{c-2}) + F_{x-2}(F_{y-1}F_{m-2}F_{b-2}F_{c-2} + F_{y-2}F_{m-3}F_{b-3}F_{c-3})] \\ &\quad + F_{x-2}(F_{y-2}F_{m-1}F_{b-1}F_{c-1} + F_{y-3}F_{m-2}F_{b-2}F_{c-2}) + F_{x-3}(F_{y-2}F_{m-2}F_{b-2}F_{c-2} + F_{y-3}F_{m-3}F_{b-3}F_{c-3}). \end{aligned}$$

Therefore, if  $k = 0$ , then  $i(H_{m,l,b,c}^k) = i(\bar{H}_{m,l,b,c}^{k,x,y})$ . If  $k > 0$ , then

$$\begin{aligned} i(H_{m,l,b,c}^k) - i(\bar{H}_{m,l,b,c}^{k,x,y}) &= 2^k F_{x-2}F_{y-2}(F_{m-1}F_{b-1}F_{c-1} - F_{m-2}F_{b-2}F_{c-2} - F_{m-3}F_{b-3}F_{c-3}) \\ &\quad + F_{x-2}F_{y-2}(F_{m-2}F_{b-2}F_{c-2} + F_{m-3}F_{b-3}F_{c-3} - F_{m-1}F_{b-1}F_{c-1}) \\ &\geq 2F_{x-2}F_{y-2}(F_{m-1}F_{b-1}F_{c-1} - F_{m-2}F_{b-2}F_{c-2} - F_{m-3}F_{b-3}F_{c-3}) \\ &\quad + F_{x-2}F_{y-2}(F_{m-2}F_{b-2}F_{c-2} + F_{m-3}F_{b-3}F_{c-3} - F_{m-1}F_{b-1}F_{c-1}) \\ &\geq F_{x-2}F_{y-2}F_{m-3}F_{b-2}F_{c-2}. \end{aligned}$$

Note that  $m \geq 3, b, c, x, y \geq 2$  and  $bc \geq 6$ , and hence  $F_{x-2}F_{y-2}F_{m-3}F_{b-2}F_{c-2} > 0$ , i.e.,  $i(\bar{H}_{m,l,b,c}^{k,x,y}) < i(H_{m,l,b,c}^k)$ . Therefore,  $i(G) \leq i(H_{m,l,b,c}^k)$ , the equality holds if and only if  $G \cong H_{m,l,b,c}^k$ .

By an argument similar to that in the proof of (a), we can also show that (b), (c) hold, respectively. This completes the proof of Lemma 2.9.  $\square$



**Fig. 5.** (i) The arrangement of seven cycles of a tricyclic graph in  $\mathcal{S}_n^7$ ; (ii) Graph  $R_{l,b,c,d}^{k,t_1,t_2}$ .

**Lemma 2.10.** For positive integers  $m, l, b, c, k$ ,

- (i)  $i(H_{m,l-1,b,c}^{k+1}) > i(H_{m,l,b,c}^k)$  for either  $l \geq 4, m \geq 3, b, c \geq 2$  and  $bc \geq 6$ , or  $l = 3, m, b, c \geq 3$ .
- (ii)  $i(H_{m-1,l,b,c}^{k+1}) > i(H_{m,l,b,c}^k)$  for  $m \geq 4, l, b, c \geq 2$  and  $lbc \geq 18$ .
- (iii)  $i(H_{m,l,b-1,c}^{k+1}) > i(H_{m,l,b,c}^k)$  for either  $b \geq 4, m \geq 3, l, c \geq 2$  and  $lc \geq 6$ , or  $b = 3, m, l, c \geq 3$ .
- (iv)  $i(H_{m,l,b,c-1}^{k+1}) > i(H_{m,l,b,c}^k)$  for either  $c \geq 4, m \geq 3, b, c \geq 2$  and  $lb \geq 6$ , or  $c = 3, l, b, c \geq 3$ .

**Proof.** (i) When  $l \geq 4, m \geq 3, b, c \geq 2$  and  $bc \geq 6$ , by Eq. (2.3) we have

$$\begin{aligned} i(H_{m,l-1,b,c}^{k+1}) - i(H_{m,l,b,c}^k) &= 2^k F_{l-4} F_{m-1} F_{b-1} F_{c-1} - F_{l-4} F_{m-2} F_{b-2} F_{c-2} + 2^k F_{l-5} F_{m-2} F_{b-2} F_{c-2} - F_{l-5} F_{m-3} F_{b-3} F_{c-3} \\ &\geq 2^k F_{l-4} F_{m-1} F_{b-1} F_{c-1} - F_{l-4} F_{m-2} F_{b-2} F_{c-2}. \end{aligned}$$

Note that  $l \geq 4, m, b, c \geq 2$ , among  $m, b, c$  at most one equal to 2, therefore,

$$2^k F_{l-4} F_{m-1} F_{b-1} F_{c-1} - F_{l-4} F_{m-2} F_{b-2} F_{c-2} > 0,$$

and so, (i) holds for  $l \geq 4, m \geq 3, b, c \geq 2$  and  $bc \geq 6$ .

When  $l = 3, m, b, c \geq 3$ , by Eq. (2.3) we have

$$\begin{aligned} i(H_{m,2,b,c}^{k+1}) - i(H_{m,3,b,c}^k) &= 2^k (2F_{m-1} F_{b-1} F_{c-1} + 2F_{m-2} F_{b-2} F_{c-2} - 2F_{m-1} F_{b-1} F_{c-1} - F_{m-2} F_{b-2} F_{c-2}) \\ &\quad + F_{m-2} F_{b-2} F_{c-2} - F_{m-2} F_{b-2} F_{c-2} - F_{m-3} F_{b-3} F_{c-3} \\ &= 2^k F_{m-2} F_{b-2} F_{c-2} - F_{m-3} F_{b-3} F_{c-3} > 0. \end{aligned}$$

This completes the proof of (i).

Similarly, we can also show that (ii), (iii) and (iv) hold, respectively.  $\square$

The following corollary follows by repeated applications of Lemma 2.10.

**Corollary 2.11.** Let  $G \in \mathcal{S}_n^6$ .

- (i) If the arrangement of its six cycles is the same as Fig. 4(I), then  $i(G) \leq i(H_{3,3,3,2}^{n-5})$ , the equality holds if and only if  $G \cong H_{3,3,3,2}^{n-5}$ .
- (ii) If the arrangement of its six cycles is the same as Fig. 4(II), then  $i(G) \leq i(Q_{3,3,3}^{n-5})$ , the equality holds if and only if  $G \cong Q_{3,3,3}^{n-5}$ .
- (iii) If the arrangement of its six cycles is the same as Fig. 4(III), then  $i(G) \leq i(S_{4,3,3}^{n-6})$ , the equality holds if and only if  $G \cong S_{4,3,3}^{n-5}$ .

If  $G \in \mathcal{S}_n^7$ , then the arrangement of its seven cycles is depicted in Fig. 5(i); see [5,6,14]. Let  $R_{l,b,c,d}^{k,t_1,t_2}$  be a tricyclic graph on  $n$  vertices (as shown in Fig. 5(ii)), where  $l + b + c + d + k + t_1 + t_2 = n + 8$ .

Using the similar method in Lemmas 2.9–2.10, we can obtain the following results, and we omit the procedure here.

**Lemma 2.12.** Let  $G \in \mathcal{S}_n^7$  such that the arrangement of its seven cycles is the same as Fig. 5(ii), then we have  $i(G) \leq i(R_{l,b,c,d}^{k,t_1,t_2})$ .

**Lemma 2.13.** Given positive integers  $l, t_1, t_2, b, c, d, k$ .

- (i)  $i(R_{l-1,b,c,d}^{k+1,t_1,t_2}) > i(R_{l,b,c,d}^{k,t_1,t_2})$  for  $l \geq 3, t_1, t_2, b, c, d \geq 2$ .
- (ii)  $i(R_{l,b-1,c,d}^{k+1,t_1,t_2}) > i(R_{l,b,c,d}^{k,t_1,t_2})$  for  $b \geq 3, l, t_1, t_2, b, c, d \geq 2$ .
- (iii)  $i(R_{l,b,c-1,d}^{k+1,t_1,t_2}) > i(R_{l,b,c,d}^{k,t_1,t_2})$  for  $c \geq 3, l, t_1, t_2, b, d \geq 2$ .
- (iv)  $i(R_{l,b,c,d-1}^{k+1,t_1,t_2}) > i(R_{l,b,c,d}^{k,t_1,t_2})$  for  $d \geq 3, l, t_1, t_2, c \geq 2$ .
- (v)  $i(R_{l,b,c,d}^{k+1,t_1-1,t_2}) > i(R_{l,b,c,d}^{k,t_1,t_2})$  for  $t_1 \geq 3, l, t_2, b, c, d \geq 2$ .
- (vi)  $i(R_{l,b,c,d}^{k+1,t_1,t_2-1}) > i(R_{l,b,c,d}^{k,t_1,t_2})$  for  $t_2 \geq 3, l, t_1, b, c, d \geq 2$ .



### 3. Main results

In this section, we determine the upper bound for the Merrifield–Simmons index of tricyclic graphs in  $\mathcal{T}_n$ , the corresponding extremal graph is characterized.

**Proposition 3.1.** *Let  $G \in \mathcal{T}_n^3$ , then  $i(G) \leq i(G_{n,3,3,3}^{n-7})$ , the equality holds if and only if  $G \cong G_{n,3,3,3}^{n-7}$ .*

**Proof.** Follows from Lemma 2.6.  $\square$

Repeated applications of Lemma 2.8 give the following proposition.

**Proposition 3.2.** *Let  $G \in \mathcal{T}_n^4$ , then  $i(G) \leq i(A_{3,3,3,2}^{n-6})$ , and the equality holds if and only if  $G \cong A_{3,3,3,2}^{n-6}$ .*

**Proposition 3.3.** *Let  $G \in \mathcal{T}_n^6$ , then  $i(G) \leq 9 \cdot 2^{n-5} + 1$ , the equality holds if and only if  $G \cong H_{3,3,3,2}^{n-5}$ .*

**Proof.** By Corollary 2.11, for any  $G \in \mathcal{T}_n^6$ ,

$$i(G) \leq \max\{i(H_{3,3,3,2}^{n-5}), i(Q_{3,3,3}^{n-5}), i(S_{4,3,3}^{n-6})\}.$$

By direct computing, we get

$$i(H_{3,3,3,2}^{n-5}) = 9 \cdot 2^{n-5} + 1, \quad i(Q_{3,3,3}^{n-5}) = 8 \cdot 2^{n-5} + 1, \quad i(S_{4,3,3}^{n-6}) = 11 \cdot 2^{n-6} + 3.$$

Once again, by Corollary 2.11,  $i(G) \leq 9 \cdot 2^{n-5} + 1$  and equality holds if and only if  $G \cong H_{3,3,3,2}^{n-5}$  for  $G \in \mathcal{T}_n^6$ .  $\square$

Repeated applications of Lemma 2.13 give the following proposition.

**Proposition 3.4.** *Let  $G \in \mathcal{T}_n^7$ , then  $i(G) \leq i(R_{2,2,2,2}^{n-4,2,2})$ , the equality holds if and only if  $G \cong R_{2,2,2,2}^{n-4,2,2}$ .*

Summarizing Propositions 3.1–3.4, we arrive at:

**Theorem 3.5.** *Let  $G \in \mathcal{T}_n$ , then  $i(G) \leq 9 \cdot 2^{n-5} + 1$ , the equality holds if and only if  $G \cong H_{3,3,3,2}^{n-5}$ .*

**Proof.** By Propositions 3.1–3.4, for any  $G \in \mathcal{T}_n$ ,

$$i(G) \leq \max\{i(G_{n,3,3,3}^{n-7}), i(H_{3,3,3,2}^{n-5}), i(A_{3,3,3,2}^{n-6}), i(R_{2,2,2,2}^{n-4,2,2})\}.$$

Note that

$$i(G_{n,3,3,3}^{n-7}) = 9 \cdot 2^{n-7} + 1, \quad i(H_{3,3,3,2}^{n-5}) = 9 \cdot 2^{n-5} + 1, \\ i(A_{3,3,3,2}^{n-6}) = 15 \cdot 2^{n-6} + 1, \quad i(R_{2,2,2,2}^{n-4,2,2}) = 8 \cdot 2^{n-5} + 1.$$

Therefore,  $i(G) \leq 9 \cdot 2^{n-5} + 1$ , by Proposition 3.3 the equality holds if and only if  $G \cong H_{3,3,3,2}^{n-5}$ .  $\square$

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